

PAPER • OPEN ACCESS

Novel method of phase determination in neutron reflectometry using reference layer

To cite this article: E S Nikova *et al* 2019 *J. Phys.: Conf. Ser.* **1389** 012153

View the [article online](#) for updates and enhancements.

Recent citations

- [A general approach to maximise information density in neutron reflectometry analysis](#)
Andrew R McCluskey *et al*



IOP | ebooks™

Bringing together innovative digital publishing with leading authors from the global scientific community.

Start exploring the collection—download the first chapter of every title for free.

Novel method of phase determination in neutron reflectometry using reference layer

E S Nikova^{1,2}, Yu A Salamatov¹, E A Kravtsov^{1,2} and V V Ustinov^{1,2}

¹M.N.Miheev Institute of Metal Physics UB RAS, S. Kovalevskoy Str. 18, Ekaterinburg, 620108, Russia

²Ural Federal University, Mira Str., 19, 620002, Ekaterinburg, Russia

E-mail: e.nikova@mail.ru

Abstract. We describe a novel method for phase recovery in neutron reflectometry which is based on using Gd reference layer of known thickness. Deposition of Gd reference layer at the top of unknown nanostructure allows us to reconstruct the complex reflection coefficient from the structure and to solve phase problem for magnetic nanostructures under investigation. This method makes it possible to use direct model-independent approaches (for example, Gelfand-Levitan-Marchenko approach) to obtain the scattering potential.

1. Introduction

The scattering of slow neutrons and, in particular, neutron reflectometry, is one of the most powerful methods for investigating the planar nanostructures, surfaces, and interlayer boundaries. The method is based on the analysis of the specular reflection of slow neutrons incident at small angles to the sample surface. This method allows us to get information about the depth dependence of neutron optical potential. Using polarized neutrons, one can also determine the depth dependence of magnetic moments.

Resonant scattering is traditionally used in X-ray reflectometry but not in neutron reflectometry because the scattering lengths of slow neutrons are generally independent of their energy. This condition is true for the most isotopes. Earlier, methods for using resonance effects in neutron diffraction have been proposed and in some cases experimentally implemented, for example, for isotopes ¹¹³Cd, ¹⁴⁹Sm, etc., to determine the amplitude and phase of wide-angle Bragg reflections [1-3]. Resonance effects in reflectometry are most often used for the analysis of secondary emission [4]. The possibilities of neutron reflectometry can be expanded by using the resonant scattering of slow neutrons by isotopic nuclei that have resonance absorption. In this paper, we use resonance effects to solve the phase problem in neutron reflectometry.

It should be noted that methods based on usage of reference layers were already developed to determine the phase of the reflection coefficient in neutron reflectometry [5-12]. These approaches are based on usage of a magnetic reference layer with known characteristics, which is deposited between unknown nonmagnetic structure and substrate. The approach implies measuring the reflection coefficient of polarized neutrons three times for every momentum transfer value (positive, negative and out-of-plane direction of magnetic field). Combined analysis of three reflectivity curves makes it possible to restore the modulus and phase of the reflection coefficient for the unknown part of the sample. In our works [13-14], we considered a possibility of usage Gd reference layer to study



magnetic multilayered structures. This is possible because two Gd isotopes, ^{155}Gd and ^{157}Gd , have a strong dependence of the scattering length versus the neutron wavelength in the thermal region [15]. Therefore, if the series of three experiments with different scattering lengths of gadolinium in the reference layer were obtained, the complex reflection coefficient of the unknown system can be determined. Earlier in numerical experiments, we showed that the method works successfully.

In this paper, the theoretical description of the proposed method is formulated. Results of an experimental determination of the modulus and phase of the complex reflection coefficient from two systems with the reference Gd layer are presented.

2. Theory

The specular reflection and transmission of neutrons in planar nanostructures is described by the Schrödinger equation

$$\frac{d^2\psi}{dz^2} + \left(\frac{Q^2}{4} - \frac{2m}{\hbar^2}V\right)\psi = 0 \quad (1)$$

where $q = \frac{4\pi \sin \theta}{\lambda}$ is momentum transfer.

Suppose that the planar nanostructure can be divided into a set of separate slices of small enough but finite thickness and scattering potential in each slice can be considered as constant.

If these equations and boundary conditions at the interface between layers i and $i-1$ are analyzed, then the amplitudes of the waves will be connected via transfer matrix

$$\begin{pmatrix} \alpha_i \\ \beta_i \end{pmatrix} = M_i \begin{pmatrix} \alpha_{i-1} \\ \beta_{i-1} \end{pmatrix} \quad (2)$$

where the transfer matrix M_i for the i -th layer of thickness d_i has the form

$$M_i = \frac{1+q_i/q_{i-1}}{2} \begin{pmatrix} e^{iq_id_i/2} & -r_i e^{-iq_id_i/2} \\ -r_i e^{iq_id_i/2} & e^{-iq_id_i/2} \end{pmatrix} \quad (3)$$

The following relationship between the reflection r and the transmission t coefficients of the nanostructure can be obtained using the continuity condition for the wave function and its derivative at the interlayer boundaries [16,17]

$$\begin{pmatrix} t \\ 0 \end{pmatrix} = M \begin{pmatrix} 1 \\ r \end{pmatrix} \quad (4)$$

Let us return to the scheme with the reference layer. In this case, the sample consists of two parts. The reflective properties are described by the matrices G and H . There is a known reference layer H on the layer G with unknown structure. This system can be considered as a two-layer and full optical matrix is

$$M = G \cdot H \quad (6)$$

The reflection coefficient r_g of the unknown part of the sample is a point on the circle in the complex plane, with radius ρ with center γ [10]:

$$\gamma = \frac{Rh_{22}h_{12}^* - h_{21}h_{11}^*}{Rh_{12}h_{12}^* - h_{11}h_{11}^*}; \quad (7)$$

$$\rho = \sqrt{R} \frac{|h_{11}h_{22} - h_{12}h_{21}|}{|Rh_{12}h_{12}^* - h_{11}h_{11}^*|}. \quad (8)$$

where h_{ij} are the elements of the matrix H , and R is the amplitude of the reflection coefficient of the complete system.

If three measurements of the reflection intensity with three different parameters of the reference layer are carried out, the reflection coefficient r_g can be defined as the intersection point of the three circles.

$$r_g = \frac{A_1(\gamma_2 - \gamma_3) + A_2(\gamma_3 - \gamma_1) + A_3(\gamma_1 - \gamma_2)}{\gamma_1^*(\gamma_2 - \gamma_3) + \gamma_2^*(\gamma_3 - \gamma_1) + \gamma_3^*(\gamma_1 - \gamma_2)}. \quad (9)$$

The coefficients A_i are related to the center γ and the radius ρ by the ratio $A_i = \gamma_i \gamma_i^* - \rho_i^2$.

3. Experiment

Firstly, the numerical simulations for model systems Cr/Fe with Gd(50Å)/V(20Å) reference layers deposited at the top of the structure were carried out. Three reflectivity curves for systems with reference layer were modeled. For each sample, the modulus and the phase of the complex reflection coefficient for initial system was calculated. Using these data the scattering potential was calculated with the Gelfand-Levitan-Marchenko equation [14].

Secondly, experiments on the neutron reflection from the non-magnetic Ti film and the three-layer film Cr/Fe/Cr with reference layer Gd(50Å)/V(50Å) were carried out. The samples were grown with UHV magnetron sputtering on Si substrates. Layer thicknesses were determined with X-ray reflectometry on PANalytical Empyrean laboratory diffractometer. The neutron reflectivity curves were measured at reflectometer REFLEX operated at IBR-2 pulsed reactor (JINR, Dubna, Russia) at three different incident angles. The polarized reflectivity curves were measured for our samples with high resolution in the Q range from 0.015 to 0.045 Å⁻¹. Background and direct beam were also measured with high resolution and good statistics.

Neutron reflectometry curves for Si//Ti(550Å)/Gd(50Å)/V(50Å) measured at three incident angles of 4.2; 5.5; 8.72 mrad are presented in figure 1.

The experimental reflectometry curves for the Si//Cr(300Å)/Fe(300Å)/Cr(200Å)/Gd(50Å)/V(50Å) three-layer systems measured at three incident angles: 3.1; 5.3; 9.0 mrad are presented in figure 2.

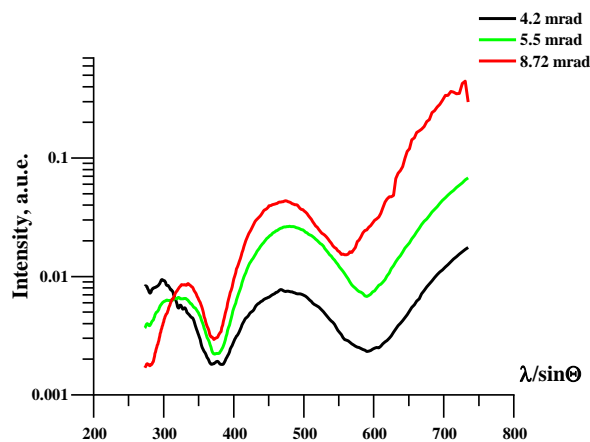


Figure 1. Reflectometry curves for Si//Ti(550Å)/Gd(50Å)/V(50Å).

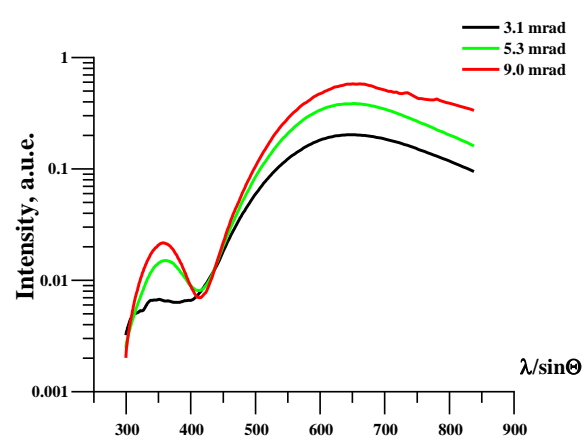


Figure 2. Reflectometry curves for Si//Cr(300Å)/Fe(300Å)/Cr(200Å)/Gd(50Å)/V(50Å).

By using equation 9 and known properties of Gd/V reference layer the modulus and phase of the complex reflection coefficient for initial systems Si//Ti(550Å) and Si//Cr(300Å)/Fe(300Å)/Cr(200Å) were calculated [18]. In figures 3 and 4 the experimentally determined modulus and phase are presented together with those calculated theoretically using nominal layer thicknesses. We note good qualitative agreement between theoretical and experimental curves.

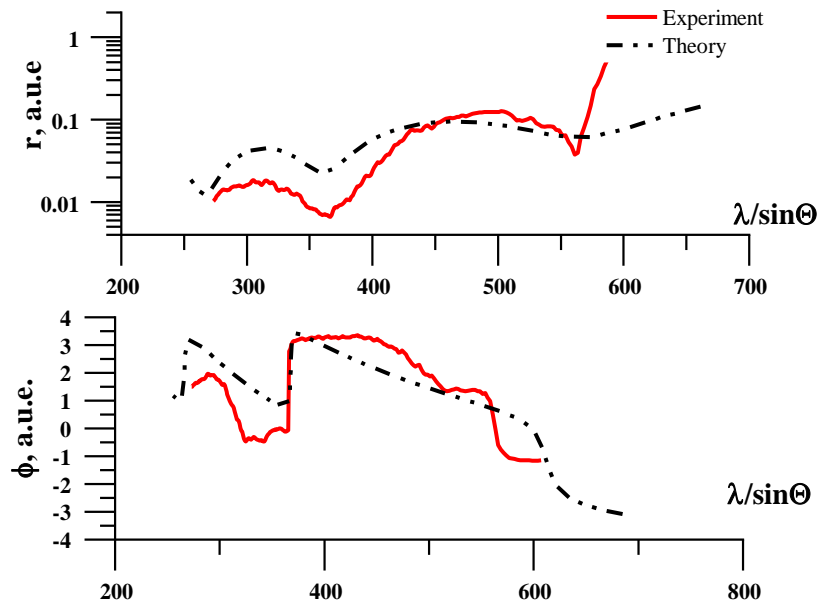


Figure 3. Modulus (a) and phase (b) of the complex reflection coefficient for the system Si//Ti(550Å).

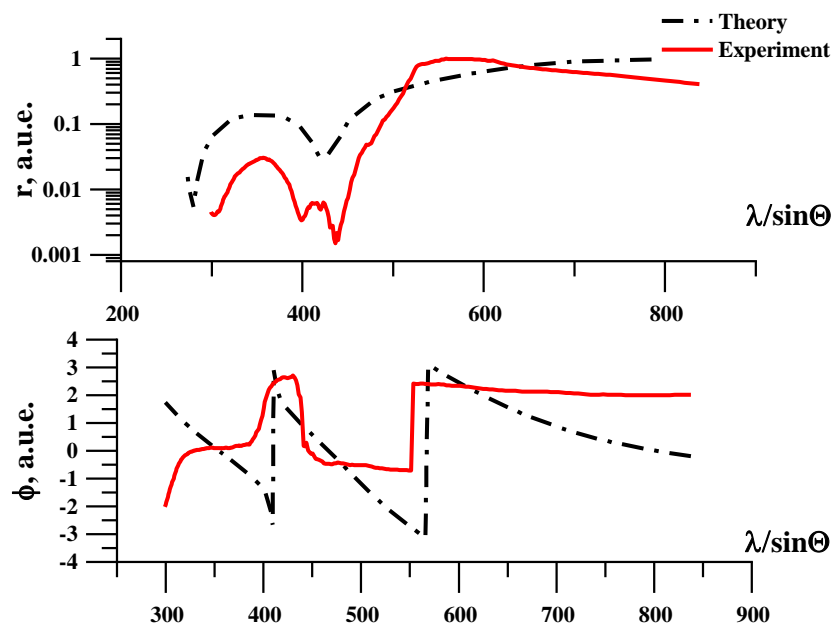


Figure 4. Modulus (a) and phase (b) of the complex reflection coefficient for the system Si//Cr(300Å)/Fe(300Å)/Cr(200Å)

4. Conclusion

It was shown that Gd reference layer deposited at the top of unknown layered structure allows us to recover the phase of complex reflection coefficient from this structure. The presented approach can be easily generalized to polarized neutrons. It gives possibility to study the magnetic nanostructures, in particular, metallic superlattices with complicated magnetic structure, e.g. with non-collinear magnetic ordering of the layers' magnetic moments.

The results showed that the phase of the reflection coefficient is most sensitive to changes of structure parameters. Small deviations of the initial values lead to significant changes in reflection phase. Thus, this allows the use of a phase to distinguish between structures having a similar reflection coefficient modulus.

Acknowledgments

The research was carried out within the state assignment «Spin» AAAA-A18-118020290104-2 and was supported in part by RFBR (project 19-02-00674).

References

- [1] Brockhouse B 1953 *Canadian J. Phys.* **31** 432
- [2] Peterson S and Smit H 1961 *Phys. Rev. Lett.* **6** 7
- [3] Smit H and Peterson S 1964 *J. Physique.* **25** 615
- [4] Nikitenko Yu 2015 *Crystallography* **60** 518
- [5] Majkrzak C and Berk N 1995 *Phys. Rev. B* **52** 10827
- [6] Majkrzak C and Berk N 1998 *Phys. Rev. B* **58** 15416
- [7] Majkrzak C, Berk N, Silin V and Meuse C 2000 *Phys. B* **283** 248
- [8] Kirby B, Kienzle P, Maranville B, Berk N, Krycka J, Heinrich F and Majkrzak C 2012 *Curr. Opin. colloid & interface Sci.* **17** 44
- [9] Majkrzak C, Carpenter E, Heinrich F and Berk N 2011 *J. Appl. Phys.* **110** 102212
- [10] de Haan V, van Well A, Sacks P, Adenwalla S and Felcher G 1996 *Phys. B* **221** 524
- [11] de Haan V, van Well A, Adenwalla S and Felcher G 1995 *Phys. Rev. B* **52** 10831
- [12] Lipperheide R, Reiss G, Leeb H, Fiedeldey H and Sofianos S 1995 *Phys. Rev. B* **51** 11032
- [13] Salamatov Yu and Kravtsov E 2016 *J. Surf. Investig. X-ray, Synchrotron Neutron Tech.* **10** 1169-72
- [14] Nikova E, Salamatov Yu, Kravtsov E and Ustinov V 2017 *Superlattices and Microstructures* **109** 201
- [15] Lynn J and Seeger P 1990 *Atomic Data and Nuclear Data Tables* **44** 191
- [16] Lekner J 1987 *Springer Science+Business Media Dordrecht* **12**
- [17] Abeles F 1950 *Ann. Physique. Paris* **5** 596
- [18] Nikova E, Salamatov Yu, Kravtsov E, Bodnarchuk V and Ustinov V 2019 *Physica B: Physics of Condensed Matter* **552** 58-61